

2,2-Dimethyl-1,3-dioxolane
2916-31-6 | DTXSID10183419

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.44×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.55×10^{-1}

Confidence level: 7.04×10^{-1}

Nearest Neighbors from the Training Set

Image not found

2,2-Dimethoxypropane

Measured: 3.92×10^{-12}

Predicted: 9.25×10^{-12}

Image not found

1,1-Dimethoxyethane

Measured: 8.89×10^{-12}

Predicted: 1.07×10^{-11}

Image not found

Diethoxymethane

Measured: 1.68×10^{-11}

Predicted: 1.95×10^{-11}

Image not found

Ethylene glycol diethyl ether

Measured: 5.79×10^{-11}

Predicted: 3.42×10^{-11}